

Analytical uncertainty propagation in life cycle inventory and impact assessment: application to an automobile front panel

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Received: 25 March 2009 / Accepted: 24 February 2010 / Published online: 8 April 2010
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Abstract

Background, aim, and scope Uncertainty information is essential for the proper use of life cycle assessment (LCA) and environmental assessments in decision making. So far, parameter uncertainty propagation has mainly been studied using Monte Carlo techniques that are relatively computationally heavy to conduct, especially for the comparison of multiple scenarios, often limiting its use to research or to inventory only. Furthermore, Monte Carlo simulations do not automatically assess the sensitivity and contribution to overall uncertainty of individual parameters. The present paper aims to develop and apply to both inventory and impact assessment an explicit and transparent analytical approach to uncertainty. This approach applies Taylor series

expansions to the uncertainty propagation of lognormally distributed parameters.

Materials and methods We first apply the Taylor series expansion method to analyze the uncertainty propagation of a single scenario, in which case the squared geometric standard deviation of the final output is determined as a function of the model sensitivity to each input parameter and the squared geometric standard deviation of each parameter. We then extend this approach to the comparison of two or more LCA scenarios. Since in LCA it is crucial to account for both common inventory processes and common impact assessment characterization factors among the different scenarios, we further develop the approach to address this dependency. We provide a method to easily determine a range and a best estimate of (a) the squared geometric standard deviation on the ratio of the two scenario scores, “A/B”, and (b) the degree of confidence in the prediction that the impact of scenario A is lower than B (i.e., the probability that $A/B < 1$). The approach is tested on an automobile case study and resulting probability distributions of climate change impacts are compared to classical Monte Carlo distributions.

Results The probability distributions obtained with the Taylor series expansion lead to results similar to the classical Monte Carlo distributions, while being substantially simpler; the Taylor series method tends to underestimate the 2.5% confidence limit by 1–11% and the 97.5% limit by less than 5%. The analytical Taylor series expansion easily provides the explicit contributions of each parameter to the overall uncertainty. For the steel front end panel, the factor contributing most to the climate change score uncertainty is the gasoline consumption (>75%). For the aluminum panel, the electricity and aluminum primary production, as well as the light oil consumption, are the dominant contributors to the uncertainty. The developed

Responsible Editor: Andreas Ciroth

Electronic supplementary material The online version of this article (doi:10.1007/s11367-010-0175-4) contains supplementary material, which is available to authorized users.

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approach for scenario comparisons, differentiating between common and independent parameters, leads to results similar to those of a Monte Carlo analysis; for all tested cases, we obtained a good concordance between the Monte Carlo and the Taylor series expansion methods regarding the probability that one scenario is better than the other.

Discussion The Taylor series expansion method addresses the crucial need of accounting for dependencies in LCA, both for common LCI processes and common LCIA characterization factors. The developed approach in Eq. 8, which differentiates between common and independent parameters, estimates the degree of confidence in the prediction that scenario A is better than B, yielding results similar to those found with Monte Carlo simulations.

Conclusions The probability distributions obtained with the Taylor series expansion are virtually equivalent to those from a classical Monte Carlo simulation, while being significantly easier to obtain. An automobile case study on an aluminum front end panel demonstrated the feasibility of this method and illustrated its simultaneous and consistent application to both inventory and impact assessment. The explicit and innovative analytical approach, based on Taylor series expansions of lognormal distributions, provides the contribution to the uncertainty from each parameter and strongly reduces calculation time.

Keywords Analytical · Climate change impact · Life cycle inventory and impact assessment · Lognormal distribution · Monte Carlo simulation · Probabilistic · Taylor series expansion · Uncertainty propagation

1 Background, aim, and scope

The present study addresses the need to provide a transparent and parsimonious decision support tool for uncertainty propagation in life cycle assessment (LCA) that can apply to both inventory and impact assessment.

Quantification and communication of uncertainties in LCA is vital for the correct interpretation and use of LCA results. In the past years, parameter uncertainty propagation has mainly been studied using Monte Carlo techniques. Hertwich et al. (1999, 2000) proposed a framework for uncertainty analysis in multimedia risk assessment and life cycle impact assessment (LCIA); they grouped the chemicals by dominant exposure route, and a Monte Carlo simulation was conducted for one representative chemical in each group. Huijbregts et al. (2003) presented a new methodology that quantifies parameter, scenario, and model uncertainty simultaneously in environmental life cycle assessment. Parameter uncertainty propagation was quantified by means of a Monte Carlo simulation, and scenario and model uncertainty were quantified by comparing

alternative scenarios and model formulations. All of the above approaches are based on Monte Carlo techniques, which are rather computationally resource intensive, especially when comparing multiple scenarios and when assessing the contributions of individual parameters. Their accuracy is often hampered by the difficulty of assigning the required uncertainty distributions to the often numerous parameters of an LCA project.

As an alternative to Monte Carlo, Heijungs (2002) and Heijungs and Suh (2002) have developed a matrix perturbation theory for uncertainty analysis. Using derivative matrices, Heijungs et al. (2005) presented an advanced analytical method for error propagation that is faster than Monte Carlo. But this method is relatively complex to apply to a case study or to the comparison of multiple scenarios.

In LCA practice, the relatively high complexity of uncertainty quantification has led to the current practice where uncertainty analysis is carried out, if at all, on the life cycle inventory (LCI) only or separately between LCI and LCIA. Since different LCA scenarios are dependent on common or correlated parameters, alternative approaches are strongly needed to enable an adequate comparison of dependent scenarios. We also need to estimate uncertainty propagation in a transparent and parsimonious way, consistently in LCI and LCIA.

An analytical and transparent uncertainty propagation method using Taylor series expansion was proposed by Morgan and Henrion (1990) and later adapted, described, and applied to a multimedia fate model by MacLeod et al. (2002). This method, hereafter referred to as the Taylor series expansion, was also used to assess the uncertainty of impact assessment models for the impacts of pesticides (Charles 2004) and to estimate the uncertainties of intake fractions (Rosenbaum et al. 2004; Rosenbaum 2006). To calculate uncertainty propagation in LCA, Ciroth et al. (2004) developed a model comparing first and higher order Taylor approximations with Monte Carlo simulations. This method shows good agreement between the two methods when the relative input uncertainty is low. For cases with medium input uncertainties, the higher order Taylor series approximation is needed, and only the Monte Carlo simulations should be used for high input uncertainties. However, their model does not discuss the specific question of scenario comparison, and therefore does not explicitly cover correlation of input variables among different scenarios, a key feature for LCA. There is also a need to illustrate the application of the Taylor series expansion method with a simple and transparent LCA case study. The objectives of the present study are (a) to further develop the Taylor series expansion method applied to lognormally based uncertainty analysis in order to be relevant for scenario comparisons and (b) to apply the developed

method in a case study to explicitly estimate uncertainty propagation simultaneously in LCI and LCIA and illustrate the simplicity of the approach. It specifically aims to answer the following questions:

1. To what extent does the Taylor series expansion method use fewer resources than Monte Carlo simulations to quantify overall uncertainty resulting from the largest sources of variance, in a way that identifies the contribution of individual parameters?
2. How can different scenarios be compared using the Taylor series expansion approach?
3. How can the Taylor series expansion be applied to both inventory and impact assessment to approximate uncertainty in way that is transparent and parsimonious while still accurate?
4. How similar are the Taylor series and Monte Carlo results for scenario comparison?

To address these challenges, we first describe and illustrate the Taylor series expansion for a single scenario and then propose a new method to extend this approach to the comparison of two or more scenarios that are dependent on common parameters. The approach is applied to an automobile case study, and resulting probability distributions are compared to those calculated by a Monte Carlo simulation. We finally discuss the potential and limitations of the Taylor series expansion compared to other methods.

2 Materials and methods

2.1 Approach for single scenario

Taylor series expansion applied to the uncertainty analysis of lognormally distributed variables

A life cycle assessment calculates the overall impact of a scenario—the output variable y —as a function of a large number of input variables x_i representing the quantities of each unit process used per functional unit, the emissions for each unit process and the impacts per unit emission: $y=f(x_1, \dots, x_n)$. Each variable can be represented by a probability distribution (e.g., normal, lognormal, or triangular). In the specific case of a lognormally distributed variable, the distribution can be characterized by a geometric mean μ and the squared geometric standard deviation GSD^2 . A GSD^2 of 2 means that 95% of the values fall between 0.5 and 2 times the geometric mean μ (see part S1 of the supporting information for basic information on lognormal distributions).

As presented in further details by Heijungs et al. (2009), the Taylor series expansion is a mathematical technique that has been applied to uncertainty analyses (Korn and Korn 1968; Morgan and Henrion 1990) to estimate the deviation

of an output variable (Δy) from the deviation of its input variables (Δx_i).

Applying the Taylor series expansion to the case where both input and output variables are lognormally distributed, section S2 of supporting information shows that the uncertainty of the output can be calculated as a function of the uncertainties of the input variables as follows:

$$\begin{aligned} & (\ln(GSD_y))^2 \\ &= \sum_{i=1}^n (\ln(GSD_{x_i}) \cdot S_i)^2 + 2 \sum_{i=1}^n \sum_{j=i+1}^n \text{Cov}[\ln x_i, \ln x_j] \cdot S_i \cdot S_j \end{aligned} \quad (1)$$

where the influence of each input parameter (i) is characterized by the following two measures:

1. The relative sensitivity (S_i) of the model output to the input parameter i describes the relative change in the model output (Δy) due to the relative change in the input parameter i (Δx_i) from the mean \bar{x} : $S_i = \frac{\partial \ln y}{\partial \ln x_i} = \left[\frac{\partial y/y}{\partial x_i/x_i} \right] \bar{x}$. An S_i of 0.5 means that for a change in input variable of 1%, the output varies by 0.5%.
2. The squared geometric standard deviation $GSD_{x_i}^2$ describes the uncertainty of parameter x_i .

Since Eq. 1 only calculates an estimate for the standard deviation, the geometric mean μ_y of the output distribution must also be calculated. Assuming that the deterministic value of the output corresponds to the mean of the output distribution \bar{y} , the geometric mean is given by (Heijungs and Frischknecht 2005) as $\mu_y = \exp(\ln(\bar{y}) - (\ln(GSD_y^2))^2/8)$. Equation S4b in supporting information then gives the lognormal probability distribution for comparison to Monte Carlo results.

In the particular case where all input factors are independent from each other, this equation simplifies to the formula proposed by MacLeod et al. (2002), with the output GSD_y^2 calculated as follows:

$$\begin{aligned} (\ln GSD_y)^2 &= S_1^2 (\ln GSD_{x_1})^2 + S_2^2 (\ln GSD_{x_2})^2 + \dots \\ &+ S_n^2 (\ln GSD_{x_n})^2 \end{aligned} \quad (2)$$

When identifying dominant sources of uncertainty for a model output, neither the sensitivity nor the uncertainty of a parameter can be interpreted on its own. Only the combination of both allows a meaningful judgment of its importance for the output.

In the specific context of LCA, using a lognormal distribution has the advantage of automatically excluding several impossible scenarios, such as negative emissions or negative uses of processes, which are meaningless in most cases and could lead to erroneous uncertainty estimates.

One limitation of the lognormal assumption is the case of influential avoided processes when using system extension, in which case impacts can be negative and therefore not capable of being represented by a lognormal distribution. The need for further development of this approach for such cases will be addressed in the final discussion.

The assumption that the output variables are lognormally distributed will first be tested by comparing the squared geometric standard deviation of Eq. 1 with the Monte Carlo upper and lower 95% confidence limits on the output. We will also compare normal and lognormal quantile-quantile (QQ) plots for the Monte Carlo distribution on the climate change score of the steel scenario and perform the Shapiro-Wilk normality test on these distributions.

The assumption of parameter independence in Eq. 2 is often not met, especially when comparing scenarios, so the next section develops how this equation must be adapted to apply the Taylor series expansion for lognormal distributions to scenario comparison in LCA.

2.2 Comparison of two scenarios

2.2.1 Comparison metric

Whether using a Monte Carlo simulation or a Taylor series expansion when comparing two scenarios, it is essential to account for their dependency on a shared set of parameters (Steen 1997). Assuming independence between two scenarios that are positively correlated could overestimate the uncertainty of the difference between scenarios. In LCA applications, comparison scenarios are always dependent on some shared parameters, because many unit processes and LCIA characterization factors are common to the different scenarios. For example, electricity consumption is directly or indirectly included in every LCA, and the global warming potentials for the various greenhouse gasses are common to all scenarios. Thus, the uncertainty of the difference between scenarios must be determined by comparing scenarios in pairs (scenarios A and B) and calculating, for a given impact result, either the uncertainty of the difference in the two results (A-B) or of the ratio of the two results (A/B).

Typically, an LCA practitioner wants to know the degree of confidence in the information that the impact of scenario A is lower than B or vice versa. This can be determined by the probability that $A-B < 0$ or that $A/B < 1$. In our case of lognormally distributed results for both scenarios A and B, the ratio A/B is especially appropriate since, by definition, it is also lognormally distributed. In contrast, A-B is, by definition, not lognormally distributed as is clear from the possibility that the lower percentiles are below zero.

2.2.2 Determination of the geometric standard deviation for the A/B distribution

Assuming that A and B are both lognormally distributed, we can show that the geometric standard deviation of the A/B distribution¹ is related to the geometric standard deviation of each scenario and to the covariance between the two scenarios by the following equation:

$$(\ln \text{GSD}_{A/B})^2 = (\ln \text{GSD}_A)^2 + (\ln \text{GSD}_B)^2 - 2\text{Cov}(\ln X_A, \ln X_B) \quad (3)$$

where X_A and X_B are the sampled inputs of scenarios A and B, respectively (see section S4 of the supporting information for derivation).

The covariance is bounded by the cases of full negative and full positive correlations:

$$-1 \leq \frac{\text{Cov}(\ln X_A, \ln X_B)}{\ln \text{GSD}_A \times \ln \text{GSD}_B} \leq 1 \quad (4)$$

Thus the bounds of the squared geometric standard deviation of the $X_{A/B}$ distribution are given by the following equation:

$$\frac{\text{GSD}_A^2}{\text{GSD}_B^2} \leq \text{GSD}_{A/B}^2 \leq \text{GSD}_A^2 \text{GSD}_B^2 \quad (5)$$

In addition, when scenarios A and B are independent (i.e., the input parameters of the two are uncorrelated) $\text{Cov}(\ln X_A, \ln X_B) = 0$ and Eq. 3 becomes

$$(\ln \text{GSD}_{A/B})^2 = (\ln \text{GSD}_A)^2 + (\ln \text{GSD}_B)^2 \quad (6)$$

Scenarios A and B are usually positively correlated in LCA, except in the case of avoided processes. Assuming no negative correlations, the range of $\text{GSD}_{A/B}^2$ is bounded by the positively correlated and independent limits:

$$\frac{\text{GSD}_A^2}{\text{GSD}_B^2} \leq \text{GSD}_{A/B}^2 \leq \left\{ \exp \left[\left((\ln \text{GSD}_A)^2 + (\ln \text{GSD}_B)^2 \right)^{\frac{1}{2}} \right] \right\}^2 \quad (7)$$

In LCA, the amount of each unit process used in the two scenarios are often independent, but some processes k are

¹ Strictly, the geometric standard deviation of the output distribution y of scenario A should have been called GSD_{y_A} . To avoid multiple complex indices, we used a simplified notation without explicitly mentioning the y , implicitly meaning that $\text{GSD}_A = \text{GSD}_{y_A}$, $\text{GSD}_B = \text{GSD}_{y_B}$ and $\text{GSD}_{B/A} = \text{GSD}_{y_{A/B}}$.

common to both scenarios (indices $m+1$ to n in Eq. 8). In addition, all impact assessment characterization or damage factors are common to all scenarios. We can therefore express the $(\ln \text{GSD}_{A/B})^2$ as the sum of the contribution of independent and common parameters. The contribution of the common parameters is expressed as a function of the difference in sensitivity between scenarios A and B:

$$\begin{aligned} (\ln \text{GSD}_{A/B})^2 &= \sum_i^l S_{A_i}^2 (\ln \text{GSD}_{A_i})^2 + \sum_{j=l+1}^m S_{B_j}^2 (\ln \text{GSD}_{B_j})^2 \\ &+ \sum_{k=m+1}^n (S_{A_k} - S_{B_k})^2 (\ln \text{GSD}_{X_k})^2 \end{aligned} \quad (8)$$

where S_{A_i} , S_{B_j} , GSD_{A_i} and GSD_{B_j} are the sensitivities and the geometric standard deviations of independent processes x_i and x_j for scenarios A and B, respectively; S_{A_k} and S_{B_k} are the sensitivities of common parameters k for scenarios A and B, respectively. GSD_{X_k} is the geometric standard deviation of common parameters k for both scenarios. Interestingly, this equation is also valid in the case of avoided burden, when S_{B_k} is negative. In this case, the two sensitivities add, leading to a larger squared geometric standard deviation.

2.2.3 Testing the degree of confidence in the scenario comparison

Typically, an LCA practitioner wants to know the degree of confidence in the prediction that the impact of scenario A is lower than B or vice versa. This can be determined by the probability that $A/B < 1$. For a lognormal distribution, this probability can be calculated using the following cumulative distribution:

$$P\left(\frac{A}{B} < 1\right) = \frac{1}{2} + \frac{1}{2} \operatorname{erf}\left[\frac{-\xi_{A/B}}{\ln \text{GSD}_{A/B} \sqrt{2}}\right] \quad (9)$$

where, erf is the error function as described in supporting information, and $\xi_{A/B}$ is the mean of the variable's logarithm. According to Pollard (1979), this parameter can be calculated assuming that the deterministic result corresponds to the mean of the distribution ($\bar{x}_{A/B}$) and using the following equation:

$$\xi_{A/B} = \ln(\bar{x}_{A/B}) - \frac{(\ln(\text{GSD}_{A/B}^2))^2}{8} \quad (10)$$

The ultimate validity of the Taylor series expansion method will be tested by comparing the calculated probabilities that the impact of A is lower than that of B with the corresponding Monte-Carlo results.

2.3 Description of the LCA automobile case study: steel versus aluminum front end panels

2.3.1 Materials selection and basic assumptions

This case study considers a hypothetical front end panel for a car, which is a structural component that bears other elements and equipment such as the headlights or the radiator grill.

Three alternative materials that could satisfy the functional and production-related requirements were selected: steel, virgin aluminum, and 100% recycled aluminum. The steel component is taken as the reference material and weighs 10 kg. The corresponding weight of the aluminum component was calculated based on a constant equivalent bending stiffness per weight of material, $E^{1/3}/\rho$, where E is Young's modulus and ρ is the density (Ashby 1992). Table 1 further specifies the recycling potential for each material type, as well as their typical market costs. The material efficiency for both the steel and the aluminum parts is assumed to be 0.65 (i.e., the weight of raw materials for the steel part is $10/0.65=15.4$ kg). The fuel consumption per marginal weight change is further assumed to be equal to 0.00004 l/kg-km. Most of the data used to determine the reference flows were based on Renard et al. (1994) and Young and Vanderburg (1994).

2.3.2 Goal definition

The main function is to ensure the transport of the mounted elements over the whole life cycle of the car (overall service of 200,000 km), requiring a similar stiffness for the different materials. The functional unit is therefore one front-end panel of equivalent stiffness providing its service over 200,000 km. The system boundaries include all the processes necessary to perform the system function, including raw material extraction, manufacturing, use phase, and end-of-life treatment. Figure 1 presents a simplified process tree for the steel and aluminum base cases, with the arrows representing the climate change performances over the product life cycle. The main factors contributing to climate change scores are gasoline, for both the aluminum and steel scenarios, and aluminum primary production. As a sensitivity study, we first increase the GSD^2 of an independent parameter, the gasoline consumption, from 1.03 to 1.77 ($\text{GSD}_{\text{independent}}^2$ in Fig. 1). We then increase the GSD^2 of a parameter common to both scenarios, the direct CO_2 emission factor for gasoline consumption, from 1.1 to 2.0 ($\text{GSD}_{\text{common}}^2$ in Fig. 1).² We

² The factors 1.77 and 2.0 were chosen to result in similar values of GSD^2 on the output for each single scenario.

Table 1 Description of the steel and aluminum scenarios

Substance	Unit	Steel	Aluminum	Ecoinvent process (Frischknecht et al. 2005)
Final weight	kg	10	3.8	Steel, low alloyed at plant RER
Materials weight	kg	15.4	5.9	Aluminum primary at plant RER
Manufacturing				
Electricity	kWh	19.7	15.2	Electricity production mix UCTE
Oil	kg	2.3 ^a	1.8 ^b	Light fuel oil, burned in boiler 100 kW, non-modulating CH
Use phase				
Gasoline	L	80	30.4	Petrol unleaded at regional storage RER, direct emissions of 2.32 kgCO ₂ /kg gasoline
Recycling rate	%	0	0	

^a Final energy generated from oil is 98 MJ

^b Final energy generated from oil is 77 MJ

finally increase the GSD^2 of these two independent and common parameters simultaneously.

2.3.3 Application of the uncertainty methodologies to the LCA case study

The uncertainty of each input parameter of the LCI is characterized by a lognormal distribution, as defined by their data pedigree within the ecoinvent database (Frischknecht et al. 2005). It must be emphasized that these uncertainty distribution are based on expert judgment and are not quantitative measures of uncertainty. The corresponding GSD^2 for each parameter is provided within Simapro 6.0 in each of the ecoinvent unit processes, with 74% of all processes being characterized as lognormally distributed and 26% undefined.

The sensitivity to each parameter was calculated using Simapro 6.0, which was also used to run Monte Carlo simulations with 1,000 iterations. The relative sensitivity to the amount of each process used per functional unit was calculated based on the individual process contribution to the global warming score. The sensitivity to the emission factors was derived from the process tree displaying the global warming scores. The sensitivity to the global warming potentials was calculated based on the contribution of each greenhouse gas to the overall global warming score. For the LCIA, we have focused on climate change impacts using the IMPACT 2002+ method (Joliet et al. 2003; i.e., global warming potential (GWP)) for a time horizon of 500 years in order to approximate integration of effects over infinity. A squared geometric standard deviation of 1.35 was retained for the GWPs to reflect the 35% uncertainty indicated by IPCC 2007.

Since Simapro only allows Monte Carlo simulations on the inventory parameters and results (without including any uncertainty on the characterization factors), we first calculate and compare inventory uncertainties in both the Monte Carlo and Taylor series methods. We then recalcu-

late the Taylor series expansion, accounting for the uncertainty on LCIA characterization factors.

3 Uncertainty results and discussion

3.1 Approach for single scenarios

Table 2 illustrates the calculation of uncertainties for the climate change score of a single scenario, including both LCI and LCIA parameter uncertainty. The calculation of the additional uncertainty due to the LCIA characterization factors is straightforward, since the sensitivity to the characterization factor of substance i is given by the relative contribution of this substance i to the overall score. The additional squared geometric standard deviation is then calculated using Eq. 2 for a single scenario or the last term of Eq. 8 for a scenario comparison. In the present case study looking at climate change impacts, the additional uncertainty due to the LCIA part is minor ($GSD^2=1.02$), because the greenhouse gas impacts are dominated by CO₂. CO₂ is the reference substance for this category and therefore has a characterization factor that is by definition exactly equal to 1.

For the LCI, we compare the GSD^2 calculated by the Taylor series for each scenario to the Monte Carlo equivalent (the ratios of the upper and lower confidence limits to the geometric mean). The Taylor series yields a GSD^2 on the climate change score of 1.09 for the steel, 1.10 for the aluminum, and 1.11 for the recycled aluminum scenario (Table 3). These values are close to those obtained using Monte Carlo (Fig. 2). When either the GSD^2 of the gasoline consumption (independent) factor is increased to 1.77 or the greenhouse gas emissions (common) factor is increased to 2.0, the GSD^2 on the climate change score calculated by the Taylor expansion increases to 1.64 (see Table 3). These are similar to the factors calculated by the Monte Carlo simulations, with the Taylor series tending to

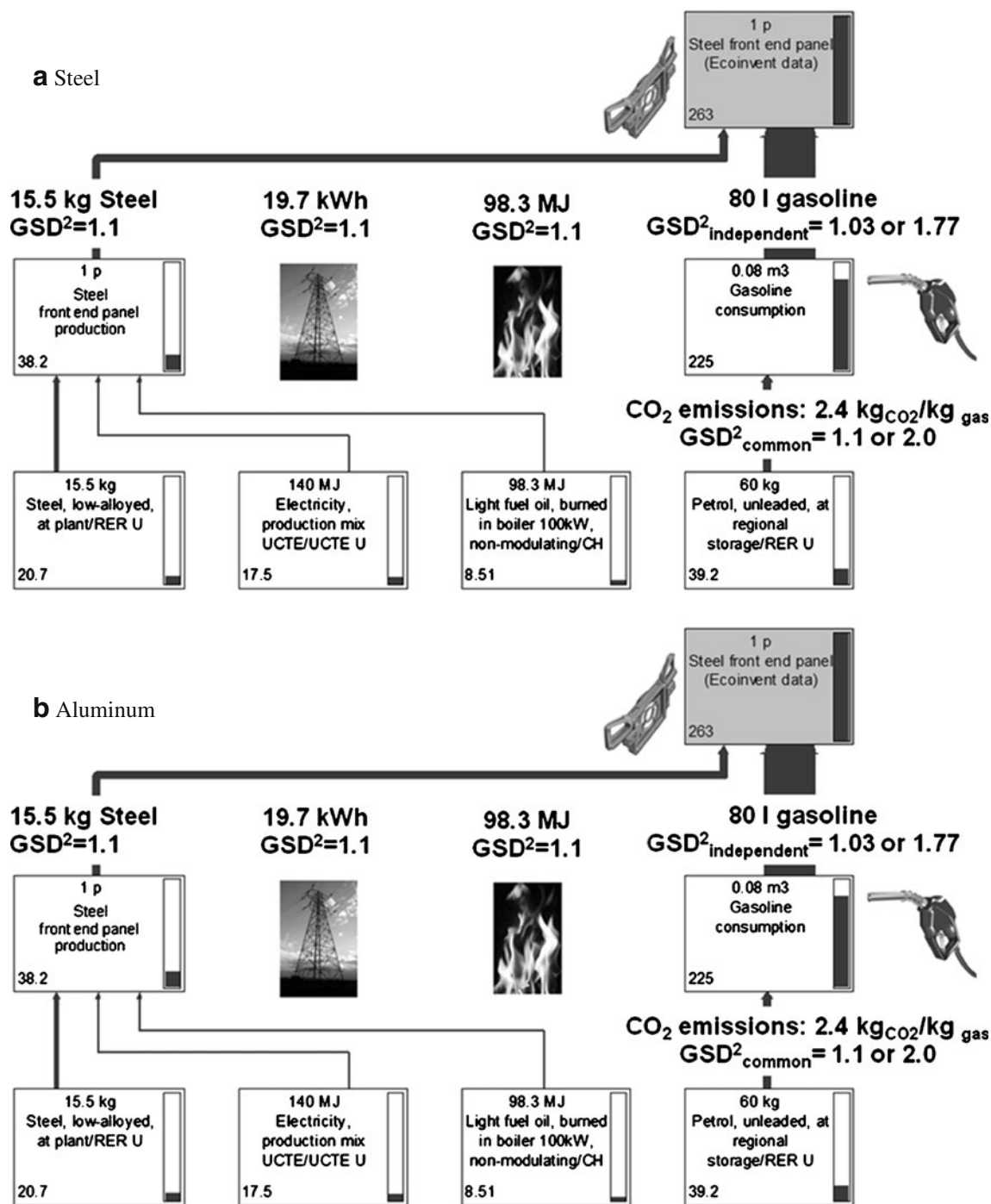


Fig. 1 Process tree and climate change impacts of the **a** steel and **b** aluminum scenarios. Associated squared geometric standard deviations on the uncertainty of the most influential parameters are also shown

slightly underestimate the 2.5% confidence limit (by 1–11%) and to a lesser extent the 97.5% upper limit (by less than 5%; see Fig. 2).

These results demonstrate the feasibility of analytical uncertainty propagation in the LCI based on a Taylor series expansion of lognormal distributions. This procedure first determines the model sensitivity to each input parameter and then assesses the overall GSD^2 on the final result as a

function of the GSD^2 of each individual input. It is fairly straightforward, while greatly reducing calculation time. Accordingly, a rapid estimation of uncertainties on large sets of LCI results can be carried out in an LCA case study.

In addition, the analytic Taylor series expansion directly provides the explicit contributions of each parameter to the overall uncertainty (Fig. 3). For the steel scenario, the factors contributing most to uncertainty of the climate

Table 2 Calculation of the squared geometric standard deviation for the aluminum scenario using the Taylor series expansion method (Eq. 2)

Process	Eco-invent database			Calculation	
	Unit	Emissions	Cf=GSD ²	Sensitivity	S _i ^{2*} (lnGSD _i) ²
Gasoline consumption	kgeq CO2	70.50	1.10	0.41	3.79E-04
Petrol, unleaded, at regional storage/RER S	kgeq CO2	14.90	1.00	0.09	0.00E+00
Hard coal, burned in power plant/DE U	kgeq CO2	9.62	1.11	0.06	8.46E-06
Aluminum, primary, liquid, at plant/RER U	kgeq CO2	8.87	1.10	0.05	6.00E-06
CF14 in Aluminum, primary, liquid, at plant/R	kgeq CO2	13.26	1.50	0.08	2.43E-04
HFC-116 in Aluminum, primary, liquid, at plant	kgeq CO2	2.97	1.50	0.02	1.22E-05
Light fuel oil, burned in industrial furnace 1 MW	kgeq CO2	7.05	2.24	0.04	2.71E-04
Light fuel oil, burned in boiler 10 kW, non-module	kgeq CO2	5.71	3.03	0.03	3.36E-04
Lignite, burned in power plant/DE U	kgeq CO2	5.34	1.11	0.03	2.61E-06
Hard coal, burned in power plant/ES U	kgeq CO2	3.81	1.11	0.02	1.33E-06
Heavy fuel oil, burned in power plant/IT U	kgeq CO2	3.00	1.09	0.02	5.61E-07
Natural gas, burned in power plant/UCTE U	kgeq CO2	2.39	1.10	0.01	4.36E-07
Hard coal, burned in power plant/FR U	kgeq CO2	1.89	1.11	0.01	3.27E-07
Hard coal, burned in power plant/IT U	kgeq CO2	1.71	1.11	0.01	2.67E-07
Operation, transoceanic freight ship/OCE U	kgeq CO2	1.64	1.05	0.01	5.37E-08
Hard coal, burned in power plant/NL U	kgeq CO2	1.57	1.11	0.01	2.25E-07
Lignite, burned in power plant/GR U	kgeq CO2	1.33	1.11	0.01	1.62E-07
Others	kgeq CO2	17.01			1.17E-03
Total LCI	kgeq CO2	172.57			2.43E-03
GSD _{LCI} ²					1.10
Affected by LCIA					
Carbon dioxide, fossil air	kgeq CO2	155.00	1.00	0.90	0.00E+00
Methane, tetrafluoro-, FC-14	kgeq CO2	13.20	1.35	0.08	1.31E-04
Ethane, hexafluoro-, HFC-116	kgeq CO2	2.98	1.35	0.02	6.69E-06
Methane, fossil	kgeq CO2	1.00	1.35	0.01	7.53E-07
Dinitrogen monoxide	kgeq CO2	0.34	1.35	1.94E-03	8.51E-08
Others	kgeq CO2	0.36	1.35	2.11E-03	1.00E-07
Total LCIA	kgeq CO2	172.88			1.39E-04
GSD _{LCIA} ²					1.02
Total GSD _{LCIA+LCI} ²					1.11

change score are the gasoline consumption, followed, to a lesser extent, by the light fuel oil consumption. In addition to these processes, the electricity production and aluminum primary production are also large sources of uncertainty for the aluminum scenario. This example demonstrates how this approach easily determines the contribution of each process to the overall uncertainty.

The lognormality hypothesis on the output variable was tested on the Monte Carlo results for the climate change score of the single steel scenarios with 10,000 simulations. The QQ plots and Shapiro-Wilk statistical tests (Shapiro and Wilk 1965) presented in part S7 of the supporting information show that the output Monte Carlo distribution is clearly closer to a lognormal distribution than to a normal distribution, with the Monte Carlo distribution even more skewed than a lognormal.

Strictly speaking, the null hypothesis that the sample is lognormally distributed is rejected by the Shapiro-Wilk test, which could be expected considering the large number of runs (10,000). This is likely due to the nature of the underlying matrix model in LCA, constituted by sums of products; the product of two lognormal distributions is lognormal but the sum is not, thus the output distribution is close to but not exactly lognormal. In practice, the Taylor expansion approach based on lognormal distributions provides a reasonable estimate of the 95% confidence interval, but tends to slightly underestimate the lower and upper confidence limits. These deviations of up to 11% and 5% seem acceptable in an LCA context for which the uncertainty distributions of the input data are defined based on expert judgment rather than on measured data.

Table 3 GSD^2 for the main input data and output climate change impacts for the aluminum and steel scenarios, and for the ratio of impacts in different scenarios, as well as the probabilities that climate change impacts from aluminum are higher than steel

	$GSD^2_{\text{on input data}}$		GSD^2_{Al}		GSD^2_{steel}			$GSD^2_{\text{steel/Al}}$		P (aluminum>steel)		
	Gasoline	Direct CO ₂ emissions	Monte Carlo ^e	Taylor	GSD^2_{steel}		Taylor	Taylor upper and lower limits (Eq.6)	Taylor indep. + common (Eq.8)	Monte Carlo	Taylor upper and lower limits (Eq.7)	Taylor indep. + common (Eq.8)
Base scenario	1.03	1.1	1.10	1.13	1.10	1.10	1.10	0.99–1.14	1.08	<0.01%	<0.00003%	<0.00003%
High $GSD^2_{\text{independent}}^a$	1.77	1.1	1.30	1.30	1.35	1.58	1.66	1.22–1.79	1.77	7.5%	0.02%–7.94%	7.54%
High $GSD^2_{\text{independent}}^b$	1.03	2.0	1.29	1.38	1.35	1.52	1.68	1.22–1.79	1.25	<0.01%	0.003%–8.32%	0.014%
High $GSD^2_{\text{independent}}$ and high $GSD^2_{\text{independent}}^c$	1.77	2.0	1.41	1.61	1.53	1.84	2.07	1.33–2.24	1.83	8.0%	0.19%–15.48%	8.82%
Base scenario with LCIA ^d	1.03	1.1	–	–	1.11	–	–	0.99–1.15	1.08	–	<0.00003%	<0.00003%

Results are shown for the base scenario, for a high GSD^2 for an independent and/or a common parameter, and for the base scenario with LCIA

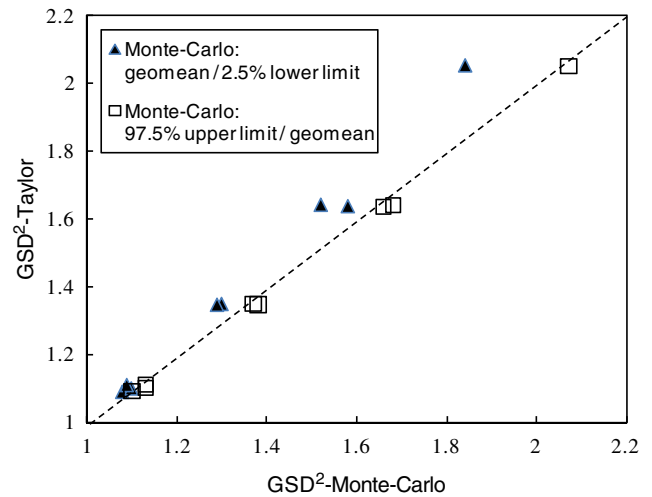
^a High uncertainty on the independent parameter gasoline consumption ($GSD^2_{\text{independent}} = 1.77$)

^b High uncertainty on the common emission factor during use phase ($GSD^2_{\text{common}} = 2.0$)

^c High uncertainty on both the independent parameter gasoline consumption and the common emission factor during use phase ($GSD^2_{\text{independent}} = 1.77$ and $GSD^2_{\text{common}} = 2.0$)

^d Base scenario including uncertainty on LCIA characterization factors

^e The Taylor series expansion GSD^2 is compared to the Monte Carlo distribution by calculating the MC ratio of the geometric mean to the 2.5% lower confidence limit (lower) and the 97.5% upper confidence limit to the geometric mean (upper)

**Fig. 2** Comparison of the squared geometric standard deviations (GSD^2) of the climate change scores of the steel, aluminum and recycled aluminum front-end panels; the Taylor series expansion approximations are compared with the equivalent Monte Carlo parameters based on 10,000 runs (the ratio of the geometric mean to the 2.5% lower confidence limit and the ratio of the 97.5% upper confidence limit to the geometric mean)

3.2 Comparison between the steel and aluminum scenarios

Figure 4 presents the Monte Carlo-based distribution of the difference between the steel and the aluminum scenarios. In this base case, the uncertainty distribution on steel-aluminum is relatively narrow and the probability that steel has a lower climate change score than aluminum is less than 0.01% ($\text{steel-aluminum} \leq 0$; Table 3). This means that the aluminum score is significantly lower than the steel one (Fig. 4a).

For our sensitivity study, we first increase the GSD^2 of an independent parameter, the gasoline consumption, for both the steel and the aluminum scenarios. This leads to a broad spread in the steel-aluminum distribution, and the probability that steel is better than aluminum ($\text{steel-aluminum} \leq 0$) increases to 7.5%, (Fig. 4b). In contrast, we can instead increase the GSD^2 of a parameter common to both scenarios, the direct CO₂ emission factor for gasoline consumption. When increasing its GSD^2 from 1.1 to 2.0, the two scenarios vary in parallel and the probability that steel is better than aluminum remains very low at <0.01% (Fig. 4c).

Using the Taylor series expansion approach, we find very similar results to Monte Carlo. The corresponding probability that steel has a lower impact than aluminum ($\text{steel/aluminum} \leq 1$) is less than 0.00003% (see Table 3), as was the case for the Monte Carlo results (less than 0.01%).

In the two sensitivity cases, each GSD^2 is bounded by the same lower and upper limits of 1.22 and 1.79 corresponding respectively to full dependency and full independency as defined in Eq. 7. The corresponding

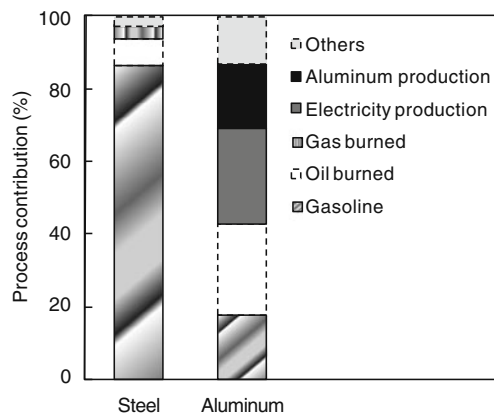


Fig. 3 Process contribution to the overall uncertainty of climate change scores calculated by the Taylor series analytical approach for steel and aluminum

probability that steel has a lower impact than aluminum ranges for both cases from 0.001% to 7.3% (see Table 3).

Accounting for the common processes between the two scenarios according to Eq. 8 enables discrimination between the independent and common cases. When increasing the $GSD^2_{\text{independent}}$ of the independent parameter from 1.03 to 1.77, the GSD^2 for the steel/aluminum ratio increases according to Eq. 8 to a high value of 1.77, corresponding to the broad distribution displayed in Fig. 5. In this case, the modified probability that steel is better than aluminum amounts to 7.0% (shaded area in Fig. 5: probability that steel/Al < 1), which is very close to the value of 7.5% obtained by the Monte Carlo method. When increasing the GSD^2_{emission} of the common parameter, the GSD^2 for the steel/aluminum ratio calculated according to Eq. 8 only amounts to 1.25, corresponding to the narrow distribution in Fig. 5. In this case, the modified probability that steel is better than aluminum is only 0.007% (no visible area under the curve below steel/Al = 1), which is close to the <0.01% observed with Monte Carlo (see Table 3). When increasing the GSD^2 of both the independent and the common parameters, the modified probability that steel is better than aluminum is close to the case of only increasing the independent parameter, for both the Monte Carlo (8%) and the Taylor expansion of Eq. 8 (8.2%).

The last row of Table 3 shows that adding the uncertainty associated with the GWP does not significantly modify the uncertainty of the steel/aluminum results compared with the base case. This is because CO_2 , which is the reference substance and therefore has a GWP equal to 1 with no associated uncertainty, is the dominant substance in this category.

If implemented in an LCA software, the Taylor series expansion method would be able to estimate uncertainties and compare scenarios quasi-instantaneously compared to

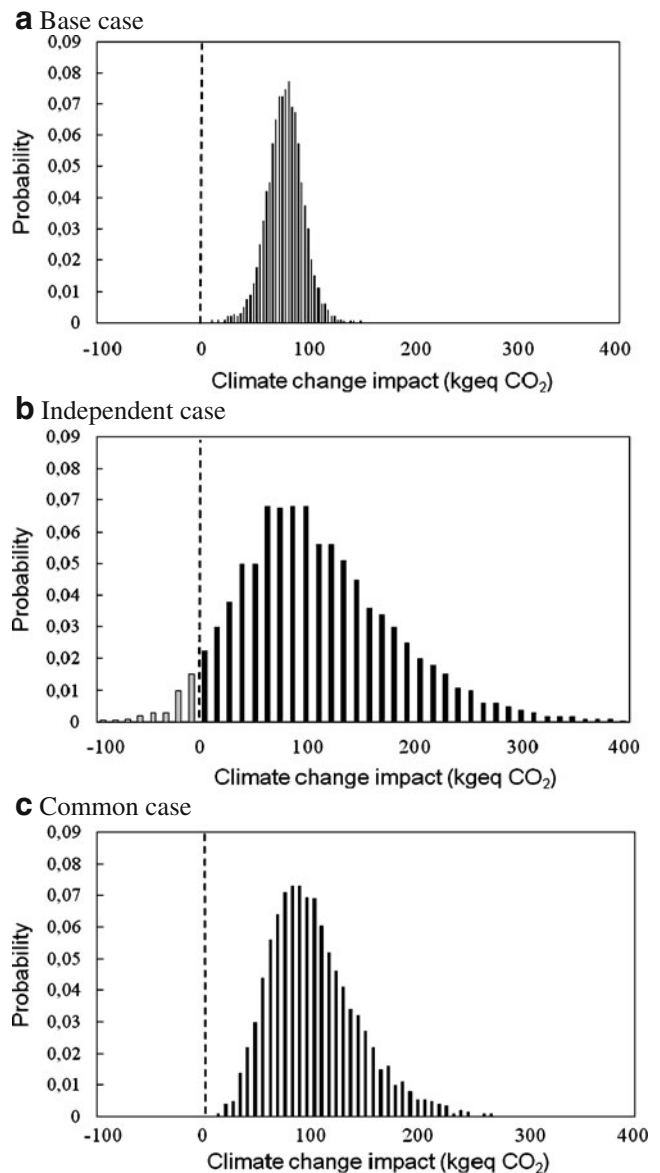


Fig. 4 Uncertainty distribution of the difference between steel and aluminum climate change impacts using Monte Carlo, with **a** base case, **b** independent case with $GSD^2_{\text{independent}} = 1.77$ varying independently between two scenarios, and **c** common case with $GSD^2_{\text{common}} = 2.0$ varying together in each simulation

the multiple hours now needed to run a Monte Carlo simulation for scenario comparison with a few thousand iterations.

4 Conclusions

First, the probability distributions obtained with the Taylor series expansion are very close to those from a classical Monte Carlo simulation, while being significantly easier to obtain. An automobile case study on an aluminum front end panel demonstrated the feasibility of this method and

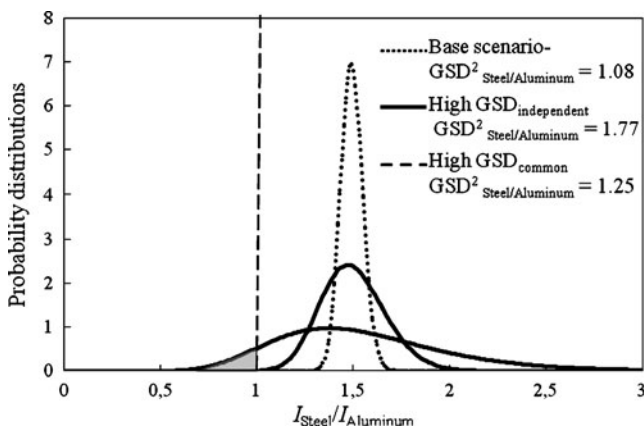


Fig. 5 Probability distributions for the ratio of steel impact score (I_{steel}) to aluminum impact score (I_{aluminum}) according to the Taylor series expansion for the base case (dotted line), for the case with high uncertainty on the independent parameter (solid line: $\text{GSD}_{\text{independent}}^2 = 1.77$) and for the high uncertainty on the common parameter (dashed line: $\text{GSD}_{\text{common}}^2 = 2.0$)

illustrated its simultaneous and consistent application to both inventory and impact assessment. We obtained for all tested cases a good concordance between Monte Carlo and the Taylor series expansion method regarding the probability that one scenario is better than the other. This indicates that despite the fact that the lognormality assumption on the output distribution is not fully met, the Taylor series expansion provides a good estimate of the degree of confidence in the comparison between scenarios. A significant advantage of the explicit analytical approach, based on Taylor series expansions of lognormal distributions, is to provide the contribution to uncertainty from each parameter in a very transparent way and strongly reduce calculation time compared to Monte Carlo analysis.

Secondly, the Taylor series expansion method addresses the crucial need of accounting for dependencies in LCA, both for common LCI processes and common LCIA characterization factors. The developed approach in Eq. 8, which differentiates between common and independent parameters, estimates the degree of confidence in the information that the impact of scenario A is lower than B, yielding results similar to those found with Monte Carlo simulations.

Finally, one limitation is that the main derivation of the presented approach is based on the assumption that the input and output parameters are approximately lognormally distributed. Such distributions are generally applicable to LCA, where factors can vary over orders of magnitude and where the lognormal assumption automatically prevents the occurrence of any meaningless negative values for LCI emission factors or LCIA characterization factors. However, having to consistently assume lognormal distributions of both input and output variables is a significant limitation with implications that must be further explored. Further work is needed to generalize the approach to various types

of distributions, for which several possibilities exist. A first-order expansion of the Taylor series can be performed on any kind of distribution (Morgan and Henrion 1990) and solved numerically, but this would not be as simple and transparent as the method presented in this paper using lognormal distributions. It would therefore be highly interesting to compare these two approaches and further study their exact domain of validity. In the same line, we need to extend the approach in order to better handle avoided impacts that could generate negative impacts, thus not covered by a lognormal distribution. Another potential improvement would consist of explicitly calculating the covariance term of Eq. 3, enabling calculation of an exact value rather than a range for the squared geometric standard deviation of the A/B distribution ($\text{GSD}_{A/B}^2$). While we expect that the simplification provided by Eq. 8 applies to most LCAs, the explicit determination of the covariance would indeed allow users to better define the domain of validity and applicability of this equation.

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